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STRONG ELECTRON TUNNELING THROUGH A SMALL METALLIC GRAIN

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Electron tunneling through mesoscopic metallic grains can be treated perturbatively only provided the tunnel junction conductances are sufficiently small. If it is not the case, fluctuations of the grain charge become strong. As a result (i) contributions of all – including high energy – charge states become important and (ii) excited charge states become broadened and essentially overlap. At the same time the grain charge remains discrete and the system conductance e-periodically depends on the gate charge. We develop a nonperturbative approach which accounts for all these features and calculate the temperature dependent conductance of the system in the strong tunneling regime at different values of the gate charge.

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Coulomb effects may have a strong impact on electron transport through small tunnel junctions and metallic grains [1, 2]. Provided the resistance of tunnel junctions R_t between the grain and the lead electrodes is large $R_t \gg R_q = \pi/2e^2 \simeq \simeq 6.5$ KΩ many features of single electron tunneling are well described within a simple perturbation theory in a dimensionless junction conductance $\alpha_t = R_q/R_t$ [1]. This theory uses the concept of discrete charge states of the grain and describe the system dynamics in terms of occupation probabilities of these charge states.

In the limit $\alpha_t \ll 1$ nontrivial features appear only in the vicinity of the Coulomb blockade threshold in which case two charge states become nearly degenerate and the perturbation theory fails. Nonperturbatively this problem has been treated in Refs. [3–5], and again the physical picture of electron tunneling via discrete charge has been exploited.

If the conductance of tunnel junctions is not small $\alpha_t > 1$ the problem turns out to be more complicated. Indeed, already making use of a simple perturbative formula for the inverse lifetime of the excited grain charge state $Q = Q_0 > e/2$ at $T = 0$ (see e.g. [1, 2]) $\Gamma = 2\alpha_t e(Q_0 - e/2)/\pi C$ one can immediately conclude that for $\alpha_t > 1$ broadening of the excited charge states $Q > e$ due to strong quantum fluctuations of the charge is of the order of the spacing between them $\Gamma \sim E_C$. Thus charge levels overlap and the very concept of tunneling via discrete charge states with given energies becomes illdefined for such values of α. The finite T effect makes this overlap even more pronounced.

In this Letter we propose a theoretical approach which allows to obtain a quantitative description of electron transport through mesoscopic metallic grains in the strong tunneling regime. We reformulate the problem in terms of the variable canonically conjugated to that of the charge, analyze its quantum dynamics and obtain an expression for the system conductance valid for all values of the gate charge and practically all experimentally relevant values of temperature.

We will consider a standard model for a SET transistor: a small metallic grain is embedded between two bulk electrodes and connected with them via tunnel junctions with resistances R_L and R_R and capacitances C_L and C_R respectively for left and right junctions. A gate voltage V_g is applied to the grain via a capacitance C_g, a transport voltage between two electrodes is equal to V_x. We also assume that the impedance of the external circuit is much less than the quantum resistance. This system can be described by the Hamiltonian

$$\hat{H} = (\hat{q} - Q_g)^2/2C + \hat{H}_L + \hat{H}_R + \hat{H}_g + \hat{H}_T, \tag{1}$$

where $\hat{q}$ is the operator of the grain charge, $Q_g = C_L V_L - C_R V_R + C_g V_g$ is the (noninteger) external charge, $V_{L,R} = V_x R_{L,R}/(R_L + R_R)$ and $C = C_L + C_R + C_g$. The terms $\hat{H}_h = \sum_k \epsilon_{kh} a^+_{kh} a_{kh}$ describe the kinetic energy of noninteracting electrons in the left ($h = L$) and right ($h = R$) electrodes and in the grain ($h = g$), whereas the term

$$\hat{H}_T = \sum_{h=L,R} \sum_{k,k'} T_h a^+_{kg} a_{k'h} \exp(-i\hat{\varphi}_h/2) + \text{c.c.} \tag{2}$$

takes care about electron tunneling between the electrodes and the grain (the tunneling matrix elements $T^{L,R}_{kk'}$ multiplied by the densities of states yield the junction resistances $R_{L,R} = 4\pi e^2 N_{L,R}(0) N_g(0) |T_{L,R}|^2$). The junctions phase operators can be expressed as

$$\hat{\varphi}_{L,R} = \frac{2eC_{R,L}}{C_L + C_R} V_x t \mp \frac{2eC_g t}{C_L + C_R + C_g} \left(\frac{C_R - C_L}{C_R + C_L} \frac{V_x}{2} - V_g \right) \mp \hat{\varphi},$$

where $\hat{\varphi}$ is the "phase" of the grain, or, more exactly, is the operator canonically conjugated to the grain charge $\hat{q}$: $[\hat{\varphi}, \hat{q}] = 2ei$.

After a standard procedure of averaging over the electronic degrees of freedom (see e.g. [2]) one can reformulate the problem in terms of the reduced density matrix $\rho(\varphi, \varphi')$ which depends only on the phase variable φ. If the charge varies continuously everywhere in the system the density matrix $\rho_c(\varphi, \varphi')$ is nonperiodic in φ [2] and obeys a standard normalization condition $\int_{-\infty}^{+\infty} d\varphi \rho_c(\varphi, \varphi) = 1$. In our physical situation, however, the charge on the grain is quantized in units of the electron charge e. In this case the phase variable is compact (i.e. the states φ and $\varphi + 4\pi$ are equivalent) and the density matrix obeys the conditions [2]

$$\rho_d(\varphi_1 + 4\pi n, \varphi_2 + 4\pi m) = \exp\left(i \frac{2\pi Q_g}{e} (n - m) \right) \rho_d(\varphi_1, \varphi_2), \tag{3}$$

$$\int_{-2\pi}^{2\pi} d\varphi \rho_d(\varphi, \varphi) = 1. \tag{4}$$

Let us now introduce a nonperiodic in φ density matrix $\tilde{\rho}(\varphi_1, \varphi_2)$:

$$\rho_d(\varphi_1, \varphi_2) = \sum_{n,m} \exp\left(i \frac{2\pi Q_g}{e} (n - m) \right) \tilde{\rho}(\varphi_1 - 4\pi n, \varphi_2 - 4\pi m), \tag{5}$$

which satisfies the following normalization condition

$$\sum_n \int_{-\infty}^{+\infty} d\varphi \exp\left(i\frac{2\pi Q_g}{e}n\right)\tilde{\rho}(\varphi - 4\pi n, \varphi) = 1. \quad (6)$$

The matrix $\tilde{\rho}$ (5) obeys the same equation of motion as the density matrix ρ_c describing the continuous charge distribution in the system. If we assume that our system is ergodic we can immediately establish the connection between these density matrices. Indeed, at sufficiently large time the solution of the linear equation of motion for a dissipative ergodic system acquire a unique form irrespectively to a particular choice of the initial conditions. Thus in the long time limit the two solutions of this equation may differ only by a constant, which can be fixed with the aid of the normalization condition and we get at $t \to \infty$

$$\tilde{\rho}(t, \varphi_1, \varphi_2) = \rho_c(t, \varphi_1, \varphi_2) / \sum_n \int_{-\infty}^{+\infty} d\varphi \exp\left(i\frac{2\pi Q_g}{e}n\right)\rho_c(t, \varphi - 4\pi n, \varphi). \quad (7)$$

The equation (7) can now be used for evaluation of the expectation value of an arbitrary operator $\hat{A}(\hat{\varphi})$, which is 4π-periodic in φ. With the aid of (5), (7) after a simple algebra we obtain

$$\left\langle \hat{A} \right\rangle_d = \int_{-2\pi}^{+2\pi} d\varphi A(\varphi)\rho_d(\varphi, \varphi) =$$

$$= \sum_n \left\langle \hat{A}(\hat{\varphi}) \exp\left(i\frac{2\pi(Q_g - \hat{q})}{e}n\right)\right\rangle_c / \sum_m \left\langle \exp\left(i\frac{2\pi(Q_g - \hat{q})}{e}n\right)\right\rangle_c. \quad (8)$$

This is one of the main results of the present paper. It establishes a straightforward connection between the expectation values for an operator of any physical quantity calculated for discrete and continuous charge distributions.

Let us now turn to a calculation of the tunneling current through a SET transistor. We first obtain a formal expression for the expectation value of the current operator in our system and then evaluate it with the aid of the equation (8). The first part of this program will be carried out within the quasiclassical Langevin Equation approach [6, 7] developed under the assumption that fluctuations of the phase variable are (in some sense) small. This is a suitable assumption as long as fluctuations of the charge are large. Expressing the kernel of the evolution operator in terms of the path integral on a real time Keldysh contour and calculating this integral within the quasiclassical approximation (see [7] for further details) we obtain

$$C_{L,R}\frac{\ddot{\varphi}_{L,R}}{2e} + \frac{1}{R_{L,R}}\frac{\dot{\varphi}_{L,R}}{2e} - \dot{q}_{L,R} = \tilde{\xi}_{R,L} = \xi_{L,R1}(t)\cos\left(\frac{\varphi_{L,R}}{2}\right) + \xi_{L,R2}(t)\sin\left(\frac{\varphi_{L,R}}{2}\right) \quad (9)$$

where $\dot{\varphi}_{L,R}/2e$ and $\dot{q}_{L,R}$ define respectively fluctuating voltages and currents across the left and the right junctions, $\xi_{L,R1,2}$ are Gaussian stochastic variables describing the shot noise in these junctions and obeying the conditions

$$\langle \xi_{R,L1,2}(0)\xi_{R,L1,2}(t)\rangle = \frac{1}{R_{R,L}}\int \frac{d\omega}{2\pi}\omega \coth\left(\frac{\omega}{2T}\right)\exp(i\omega t).$$

As the external impedance is negligible, the phases $\varphi_{L,R}$ are linked to the transport voltage V_x by means of an obvious equation $\dot{\varphi}_L + \dot{\varphi}_R = 2eV_x$. Further relations between the phase and the charge variables are defined by the charge conservation law $\dot{q}_L - \dot{q}_R = C_g\ddot{\varphi}_g/2e$ and the Kirghoff's law $\dot{\varphi}_L/2e - \dot{\varphi}_R/2e = 2V_g - \dot{\varphi}_g/e$, φ_g is the gate capacitance phase defined analogously to $\varphi_{L,R}$. Combining all these equations with (9) after averaging over the stochastic variables ξ we arrive at the expression for the current in our system:

$$I = \langle \dot{q}_L \rangle = \frac{V_x}{R_L + R_R} - \frac{R_L \langle \tilde{\xi}_L \rangle_d + R_R \langle \tilde{\xi}_R \rangle_d}{R_L + R_R}. \tag{10}$$

To evaluate the average values in (10) we shall use the result (8). Assuming that fluctuations of the charge are Gaussian the contribution of the n-th term to the expectation value (8) can be roughly estimated as:

$$\left\langle A(\varphi)\exp\left(i\frac{2\pi q}{e}n\right)\right\rangle_c \sim \exp\left(-\frac{2\pi^2 \langle \delta q^2 \rangle}{e^2}n^2\right). \tag{11}$$

Thus provided the charge fluctuations are not small $\langle \delta q^2 \rangle > e^2$ it is sufficient to leave only the terms with $n, m = 0, \pm 1$ in the expression (8). In this approximation we obtain

$$\langle \tilde{\xi}_{R,L} \rangle_d = \frac{\langle \tilde{\xi}_{R,L} \rangle + 2\langle \tilde{\xi}_{R,L} \cos\left(\frac{2\pi}{e}q\right)\rangle}{1 + 2\langle \cos\left(\frac{2\pi}{e}q\right)\rangle}, \tag{12}$$

where $\langle ... \rangle$ denotes the average with the density matrix ρ_c describing the continuous charge distribution. Making use of the equations (10), (12) and assuming the phase fluctuations to be small $|\delta\varphi| < \pi$ in the limit of small transport voltages we arrive at the expression for the linear conductance

$$(R_L + R_R)G(T) = 1 - f(T) - g(T)e^{-F(T)}\cos\left(\frac{2\pi Q_g}{e}\right), \tag{13}$$

where $Q_g = C_g V_g$. We define $\alpha_t = \pi/2e^2 R_0$, $1/R_0 = 1/R_L + 1/R_R$ and

$$f(T) = \frac{1}{2\alpha_t}\left[\gamma + \frac{2\alpha_t E_C}{\pi^2 T}\Psi'\left(1 + \frac{2\alpha_t E_C}{\pi^2 T}\right) + \Psi\left(1 + \frac{2\alpha_t E_C}{\pi^2 T}\right)\right], \tag{14}$$

$$\begin{aligned} F(T) = \frac{2\pi^2\langle \delta q^2(T)\rangle}{e^2} &= \frac{\pi}{e^2 R_0}\int_{-\infty}^{+\infty} dx \frac{x \coth(x/2TR_0C)}{1 + x^2} = \\ &= F(0) + \frac{\pi^2 T}{E_C} + 4\alpha_t\left(\ln\left(\frac{2\alpha_t E_C}{\pi^2 T}\right) - \Psi\left(1 + \frac{2\alpha_t E_C}{\pi^2 T}\right)\right), \end{aligned} \tag{15}$$

$$g(T) = \frac{2e^2}{\pi}\int_0^{+\infty} dt \left(\frac{\pi T}{\sinh \pi T t}\right)^2 t\left(K(t)(\cosh u(t) - 1) + \frac{2\pi C}{e^2}\dot{K}(t)\sinh u(t)\right). \tag{16}$$

Here $\Psi(x)$ is the logarithm of the gamma-function, $\gamma = 0.577...$ is the Euler constant and

$$\begin{aligned} K(t) &= R_0\theta(t)(1 - \exp(-t/R_0C)), \\ u(t) &= R_0 C \int d\omega \frac{\coth(\omega/2T)\sin\omega t}{1 + \omega^2 R_0^2 C^2}. \end{aligned} \tag{17}$$

Note that the value $F(0) \propto \langle \delta q^2(0) \rangle$ (15) diverges logarithmically at high frequencies. As in the small voltage limit the Langevin equation approach does not work at very low T (see below), in order to define $F(0)$ (or, equivalently, the high frequency cutoff for (15)) we should make use of a more rigorous technique. For $V_x = 0$ we find

$$\left\langle \cos \frac{2\pi \hat{q}}{e} \right\rangle = \frac{\int d\varphi \rho_{\rm eq}(4\pi + \varphi, \varphi)}{\int d\varphi \rho_{\rm eq}(\varphi, \varphi)} \cos \frac{2\pi Q_g}{e},$$

$\rho_{\rm eq}(\varphi, \varphi')$ is the equilibrium density matrix of our system. In the limit $\alpha_t > 1$ this matrix was evaluated by means of various nonperturbative approaches [8, 9]. In the leading order in $e^{-2\alpha_t}$ all these approaches yield

$$\frac{\int d\varphi \rho_{\rm eq}(4\pi + \varphi, \varphi)}{\int d\varphi \rho_{\rm eq}(\varphi, \varphi)} = e^{-2\alpha_t}.$$

Thus we obtain

$$F(0) \simeq 2\alpha_t. \tag{18}$$

This equation completes our results. In the limit of large T the Q_g – dependent part of the conductance vanishes and we find the asymptotic behavior:

$$(R_R + R_L)G(T) = 1 - \frac{E_C}{3T} + \frac{6\zeta(3)}{\pi^4}\alpha_t \left(\frac{E_C}{T}\right)^2 - \ldots \tag{19}$$

At lower temperatures the conductance suppression due to charging effects becomes more pronounced (fig. 1). Furthermore, by changing the gate charge Q_g it becomes possible to e-periodically tune the value of G. The minimum and maximum conductance values (fig. 1) correspond to $Q_g = 0$ and $Q_g = e/2$ where the Coulomb barrier for electron tunneling reaches respectively its maximum and minimum values. The modulation of G with Q_g also becomes more pronounced as the temperature is lowered (fig. 2).

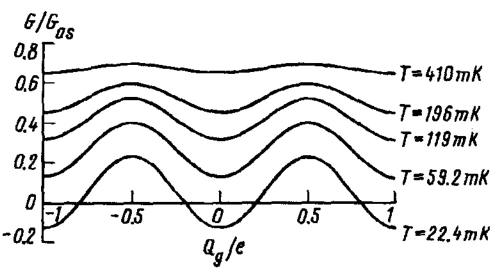

Fig.1. Maximum and minimum conductance versus temperature ($E_C = 0.715$K, $\alpha_t = 2.12$)

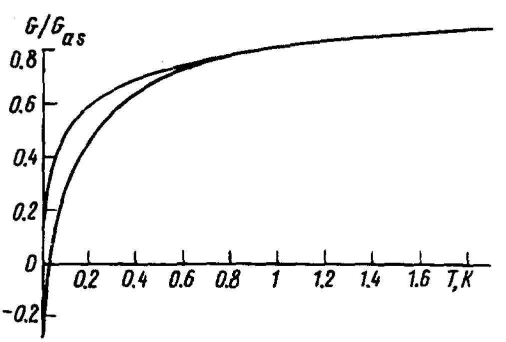

Fig.2. Dependence of conductance on gate voltage ($E_C = 0.715$K, $\alpha_t = 2.12$)

Finally, let us formulate the validity condition for our results. Analogously to [7] we find that the phase fluctuations are sufficiently small provided $T \gg E_C$ for $\alpha_t \ll 1$ and

$$T \gg \alpha_t E_C \exp(-2\alpha_t) \tag{20}$$

for $\alpha_t > 1$. Another our assumption $\langle \delta q^2 \rangle > e^2$ is also well justified for such values of T. According to (20) the validity domain of our analysis expands rapidly with increasing α_t. E.g. for the parameters of figs.1, 2 the condition (20) yields $T > 20$ mK. And indeed our results show a very good agreement with a preliminary experimental data of the Saclay group[1)] down to such small values of T.

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